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STepwise Magnetic Behavior of the Liquid Crystal Iron(Iii) Complex

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Abstract

EPR and Mossbauer spectroscopy is used to study a new liquid crystal complex of iron(III) with a Schiff base: 4,4'S-dodecyloxybenzoyloxybenzoyl-4- oxysalicylidene-2-aminopyridine with a PF6'{ counterion. It is shown that Fe(III) ions exist only in the high-spin (HS, S = 5/2) state. It is found that under the influence of temperature the system demonstrates the stepwise behavior of the product of the integrated intensity of EPR lines (I) and temperature (proportional to "where" is the magnetic susceptibility) with an inflection point at "80 K. Above 80 K a new EPR spectrum is detected due to the excited S = 2 state and the formation of dimeric molecules (through oxygen bridges) with a strong intramolecular antiferromagnetic exchange interaction J1 = 162.1 cm-V1. Below 80 K iron(III) complexes are organized in 1D chains where the exchange value J2 = 2.1 cm-V1. At 80 K there is a structural phase transition in the system: the transition from a 1D chain organization of HS Fe(III) centers to dimeric molecules. Based on quantum chemical calculations a model of the binuclear iron(III) complex is proposed. Copyright © 2013 by N. E. Domracheva, V. E. Vorob'eva, A. V. Pyataev, R. A. Manapov, E. M. Zueva, M. S. Gruzdev, U. V. Chervonova.

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Keywords

DFT., Electron paramagnetic resonance (EPR), Fe(III) complexes, Liquid crystals, M'Ssbauer spectroscopy, Magnetic properties, Quantum chemical calculations, Schiff bases, Spin-crossover